On the roots of certain polynomials arising from the analysis of the Nelder–Mead simplex method

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Abstract

The study of the effect of dimensionality on the Nelder–Mead simplex method for unconstrained optimization leads us to the study of a two parameter family of polynomials of the form

\[ p_n(z) = b - az - \cdots - az^{n-1} + z^n, \]

where \( a, b \in \mathbb{C} \). We show that provided that \( \bar{a} - ab \) is real, it is possible to use, primarily, the Schur–Cohn Criterion in order to determine the configuration of the roots of \( p_n(z) \) with respect to the unit circle.

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1. Introduction

In this paper we study the location with respect to the unit circle of the roots of a two-parameter family of polynomials of the following form:

\[ p_n(z) = b - az - \cdots - az^{n-1} + z^n, \quad a, b \in \mathbb{C}. \] (1.1)

Such polynomials arise in the theoretical analysis of the convergence of the Nelder–Mead simplex algorithm which is a widely used method for solving unconstrained optimization problems. For a detailed description of the algorithm, see [7,9].

An important question in the theoretical analysis of the Nelder–Mead method is the effect of dimensionality on the method, see [7,10]. In [3] it was found that we can gain much insight into the behavior of the Nelder–Mead method by considering the quadratic function

\[ x_1^2 + x_2^2 + \cdots + x_n^2. \]

For certain choices of the initial simplex

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and when one type of step (inside contraction, outside contraction, or reflection) is applied repeatedly, we can establish recurrence relations for the vertices of successive simplices. The characteristic polynomials of these recurrence relations are of the form (1.1) with

In the case of inside contraction: \( a = \frac{1}{2^n}, \ b = -\frac{1}{2} \), \hfill (1.2)

In the case of outside contraction: \( a = \frac{3}{2^n}, \ b = \frac{1}{2} \), \hfill (1.3)

and

In the case of reflection: \( a = \frac{2}{n}, \ b = 1 \), \hfill (1.4)

respectively.

From the point of view of the convergence of the method, it is expected that all the roots of the characteristic polynomials arising from the inside contraction and the outside contraction steps to lie in the interior of the unit disk and for all the roots of the characteristic polynomial arising from the reflection steps to be located on the unit circle. We shall prove these facts in Sections 3 and 4. Moreover, we are concerned with the effect of dimensionality on the Nelder–Mead method as \( n \) becomes large. In Section 5, we shall consider how the roots of these characteristic polynomials behave as \( n \) increases.

There are a number of results in the literature that allow us to conclude a certain portion of our findings here. We give two examples. Let

\[
g_n(z) = a_0 + a_1 z + \cdots + a_{n-1} z^{n-1} + z^n. \tag{1.5}
\]

Then according to Householder [6, Exercise 5, p. 73], if \( a_0 \neq 0 \), then no root of \( g_n \) is less in modulus than the positive root of the polynomial

\[
q_n(z) = -|a_0| + |a_1| z + \cdots + |a_{n-1}| z^{n-1} + z^n. \tag{1.6}
\]

Furthermore, Householder [6, Exercise 11, p.73], quotes a result, most probably due to Ostrowski, that no root of \( g_n \) exceeds \( 2 \max_{0 \leq j \leq n-1} \{|a_j|^{1/j}\} \). We shall explain, and give examples of, how our results refine the deductions that can be made from the aforementioned results as they pertain to (1.1).

There are yet further results in the literature concerning the location of roots of polynomials. For example, Theorems 42.1 and 44.1 of [8] deal with the location of roots with respect to the unit circle for the general polynomial

\[
h_n(z) = a_0 + a_1 z + \cdots + a_n z^n. \tag{1.7}
\]

An alternative theorem to Theorem 42.1 of [8] is the so called Schur–Cohn Criterion which is a very useful tool for determining the number of roots of polynomial (1.7) lying inside the unit circle. In Section 2 we shall state the Schur–Cohn Criterion and derive some useful conclusions for polynomials of the form (1.1).
To carry out our analysis we shall assume that $a$ and $b$ in (1.1) satisfy that
\[ \Im(\bar{a} - a\bar{b}) = 0, \tag{1.8} \]
where $\Im(\cdot)$ denotes the imaginary part of a complex number. Under these conditions, but particularly when $a, b \in \mathbb{R}$, we shall show that the roots of (1.1) must have one of the following configurations with respect to the unit circle:

- All the roots lie in the interior of the unit disk.
- All the roots lie in the exterior of the unit disk.
- $n-1$ of the roots lie in the interior of the unit disk.
- $n-1$ of the roots lie in the exterior of the unit disk.
- All the roots lie on the unit circle.
- $n-1$ of the roots lie on the unit circle and one root lies in the interior of the unit disk.

In Section 3 we shall consider the cases of $a, b \in \mathbb{C}$, but especially in $\mathbb{R}$, satisfying (1.8) or, which result in no roots of (1.1) lying on the unit circle, whereas in Section 4, we shall consider such $a$’s and $b$’s which lead to some: 1, or $n-1$, or $n$ roots on the unit circle. In Section 5, we shall show that the roots of the characteristic polynomials for inside contraction and outside contraction converge to the boundary of the unit circle.

2. The general problem via Schur–Cohn

Consider the two parameter family of polynomials given in (1.1). In this section we shall apply the Schur–Cohn Criterion for the location of its roots relative to the unit circle for a wide range of values of the parameters $a$ and $b$.

Let us begin with the general polynomial
\[ h_n(z) = a_0 + a_1 z + \cdots + a_n z^n. \tag{1.7} \]

The Schur–Cohn Criterion can be stated as follows:

**Lemma 2.1** (Marden [8, Theorem 43.1, p. 152]). For the polynomial $h_n(z)$ given in (1.7), define
\[ A_k := \det \begin{bmatrix} A_k^* & A_k^{*H} \\ A_k^H & A_k^{H*} \end{bmatrix}, \quad k = 1, 2, \ldots, n, \tag{2.1} \]
where
\[ A_k := \begin{bmatrix} a_0 & 0 & 0 & \cdots & 0 \\ a_1 & a_0 & 0 & \cdots & 0 \\ a_2 & a_1 & a_0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{k-1} & a_{k-2} & a_{k-3} & \cdots & a_0 \end{bmatrix}. \]
\[ A_k^* := \begin{bmatrix}
\bar{a}_n & 0 & 0 & \cdots & 0 \\
\bar{a}_{n-1} & \bar{a}_n & 0 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\bar{a}_{n-k+1} & \bar{a}_{n-k+2} & \bar{a}_{n-k+3} & \cdots & \bar{a}_n
\end{bmatrix}, \]

and \( B^H := \bar{B}^T \) for any matrix \( B \).

If \( A_k \neq 0, \quad k = 1, 2, \ldots, n, \)
then \( h_n(z) \) has no zeros on the unit circle and the number of its zeros inside this circle is equal to the number of negative elements in the sequence
\[
A_1, \ A_2/A_1, \ldots, A_n/A_{n-1}. \tag{2.2}
\]

Using the Schur–Cohn Criterion we shall first derive conditions on how many roots of \((1.1)\) lie inside or outside the unit circle. Indeed, assuming that \( a, b \in \mathbb{C} \), we have that here
\[
A_k := \begin{bmatrix}
b & 0 & 0 & \cdots & 0 \\
-a & b & 0 & \cdots & 0 \\
-a - a & b & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-a - a & -a & \cdots & b
\end{bmatrix}
\]

and
\[
A_k^* := \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
-\bar{a} & 1 & 0 & \cdots & 0 \\
-\bar{a} - \bar{a} & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
-\bar{a} - \bar{a} & -\bar{a} & \cdots & 1
\end{bmatrix}, \tag{2.5}
\]

It can be readily verified that the matrices \( A_k^* \) and \( A_k \) commute. Therefore, using a matrix factorization \([5, \text{p. } 17]\), we have that
\[
A_k = \det(Q_k), \tag{2.3}
\]
where
\[
Q_k = A_k A_k^H - A_k^* A_k^{*H}. \tag{2.4}
\]

By a straightforward calculation we get that
\[
Q_k = (|b|^2 - 1)I + H_k, \tag{2.5}
\]
where
\[
H_k := \begin{bmatrix}
0 & a - \bar{a}b & \cdots & a - \bar{a}b \\
\bar{a} - a\bar{b} & 0 & \cdots & a - \bar{a}b \\
\vdots & \vdots & \ddots & \vdots \\
\bar{a} - a\bar{b} & \bar{a} - a\bar{b} & \cdots & 0
\end{bmatrix}. \tag{2.6}
\]
Notice that $H_k$ is an Hermitian matrix with zero diagonal entries and with identical entries in the strictly lower triangular part and hence also with identical entries in its strictly upper triangular part, the latter being, of course, the conjugates of the former.

If the coefficients $a$ and $b$ of the polynomial in (1.1) satisfy (1.8), namely, that $\Im(\bar{a} - a\bar{b}) = 0$, then the eigenvalues of $Q_k$ of (2.5) are $((|b|^2 - 1) - (\bar{a} - a\bar{b}))$ with multiplicity $k - 1$ and $((|b|^2 - 1) + (k - 1)(\bar{a} - a\bar{b}))$ with multiplicity 1 and we immediately arrive at the following conclusion:

**Observation 2.2.** Let $Q_k$ and $H_k$ be the matrices given in (2.5) and (2.6). If $\Im(\bar{a} - a\bar{b}) = 0$, then

$$A_k = \det(Q_k) = [(|b|^2 - 1) - (\bar{a} - a\bar{b})]^{k-1}[(|b|^2 - 1) + (k - 1)(\bar{a} - a\bar{b})].$$

We shall use this observation along with the Schur–Cohn Criterion to characterize the location of roots of polynomial (1.1) with respect to the unit circle. We comment, though, that when $\Im(\bar{a} - a\bar{b}) /\neq 0$, then it is still possible to obtain an explicit formula for the eigenvalues of $H_k$, and hence also for $Q_k$, via a result due to Elsner [1, p. 35] which gives the eigenvalues of an $n \times n$ matrix $G$ whose entries $g_{i,j}$ satisfy that $g_{i,i} = 0$, $i = 1, \ldots, n$, $g_{i,j} = r$, $1 \leq j < i \leq n$, and $g_{i,j} = s$, $1 \leq i < j \leq n$, for some arbitrary but fixed constants $r$ and $s$.

We conclude this section by applying Observation 2.2 to express, when $\Im(\bar{a} - a\bar{b}) = 0$ and $\bar{a} - a\bar{b} /\neq 0$, the ratios in the sequence (2.2), where the $A_k$'s are given in (2.1). We see that

$$A_1 = |b|^2 - 1,$$

and

$$A_k/A_{k-1} = \frac{1-|b|^2}{a-ab} + 1 \quad \frac{1-|b|^2}{a-ab} - (k-1) \quad (\bar{a}\bar{b} - \bar{a}),$$

$$k = 2, 3, \ldots, n.$$  \hspace{1cm} (2.7)

Thus, when $\Im(\bar{a} - a\bar{b}) = 0$ and $\bar{a} - a\bar{b} /\neq 0$, it suffices to check the sign pattern of the above sequence so as to determine how the roots of (1.1) are distributed with respect to the unit circle.

### 3. The case of no roots on the unit circle

In this section we consider conditions on $a, b \in \mathbb{C}$, but especially in $\mathbb{R}$, which satisfy (1.8) and which ensure that no root of (1.1) lies on the unit circle. In the following lemma, we shall state and prove the results when $a$ and $b$ are real and then, in a subsequent remark we shall address the complex case.
Lemma 3.1. Suppose that \( a, b \in \mathbb{R}, \ a(b - 1) \neq 0, \ |b| \neq 1, \) and \( (b + 1)/a \neq k, \) where \( k = -1, 0, 1, 2, \ldots, n - 1. \) Then

I Assuming that \( a(b - 1) < 0: \)
\[ \text{I.i} \quad \text{When } |b| < 1: \]
\[ \text{I.i.1} \quad \text{The polynomial in (1.1) has all its roots in the interior of the unit disk if} \]
\[ \frac{b + 1}{a} > n - 1. \quad (3.1) \]
\[ \text{I.i.2} \quad \text{The polynomial in (1.1) has } n - 1 \text{ roots in the interior of the unit disk and one root in its exterior if} \]
\[ 0 < \frac{b + 1}{a} < n - 1, \text{ but } \frac{b + 1}{a} \notin \mathbb{Z}. \]

\[ \text{I.ii} \quad \text{When } |b| > 1: \]
\[ \text{I.ii.1} \quad \text{The polynomial in (1.1) has all its roots in the exterior of the unit disk if} \]
\[ \frac{b + 1}{a} < -1. \]
\[ \text{I.ii.2} \quad \text{The polynomial in (1.1) has } n - 1 \text{ roots in the exterior of the unit disk and one root in its interior if} \]
\[ -1 < \frac{b + 1}{a} < 0. \]

II Assuming that \( a(b - 1) > 0: \)
\[ \text{II.i} \quad \text{When } |b| < 1: \]
\[ \text{II.i.1} \quad \text{The polynomial in (1.1) has all its roots in the interior of the unit disk if} \]
\[ \frac{b + 1}{a} < -1. \quad (3.2) \]
\[ \text{II.i.2} \quad \text{The polynomial in (1.1) has } n - 1 \text{ roots in the exterior of the unit disk and one root in its interior if} \]
\[ -1 < \frac{b + 1}{a} < 0. \]

\[ \text{II.ii} \quad \text{When } |b| > 1: \]
\[ \text{II.ii.1} \quad \text{The polynomial in (1.1) has all its roots in the exterior of the unit disk if} \]
\[ \frac{b + 1}{a} > n - 1. \]
\[ \text{II.ii.2} \quad \text{The polynomial in (1.1) has } n - 1 \text{ roots in the exterior of the unit disk and one root in its interior if} \]
\[ 0 < \frac{b + 1}{a} < n - 1, \text{ but } \frac{b + 1}{a} \notin \mathbb{Z}. \]
Proof. Since $a, b \in \mathbb{R}$, the ratios (2.7) can be rewritten as

$$
A_k/A_{k-1} = \frac{\left(\frac{b+1}{a} + 1\right)\left(\frac{b+1}{a} - (k - 1)\right)}{\frac{b+1}{a} - (k - 2)} a(b - 1), \quad k = 2, 3, \ldots, n. \quad (3.3)
$$

The conditions $a(b - 1) \neq 0$, $|b| \neq 1$, and $(b + 1)/a \neq k$ (for $k = -1, 0, 1, 2, \ldots, n$) guarantee that $A_k \neq 0$, for $k = 1, 2, \ldots, n$. Thus the Schur–Cohn Criterion (Lemma 2.1) can be applied for the location of roots of polynomial (1.1).

We can now proceed by checking the sign pattern of the sequence in (2.2) to determine how the roots of (1.1) are located with respect to the unit circle. Let us take Case I.i.2 as an example, all other cases can be checked similarly. In this case, there exists exactly one ratio positive in (3.3) because there is exactly one $k \in \{2, 3, \ldots, n\}$ such that $k - 2 < (b + 1)/a < k - 1$. Therefore, in Case I.i.2, we have that $A_1 = b^2 - 1 < 0$, $n - 2$ ratios in (3.3) are negative, and one is positive. Using the Schur–Cohn Criterion, we conclude that the polynomial in (1.1) has $n - 1$ roots in the interior of the unit disk and one root in its exterior. □

Remark 3.2. We can extend Lemma 3.1 to the case when $a$ and $b$ are complex. Specifically, all the conclusions of Lemma 3.1 hold for the complex case when condition (1.8) is satisfied if we replace $(b + 1)/a$ by $(1 - |b|^2)/[\bar{a} - a\bar{b}]$ and $a(b - 1)$ by $a\bar{b} - \bar{a}$ everywhere in the lemma.

Remark 3.3. Recall now Ostrowski’s result quoted from Householder’s book following (1.6), namely, that no root of the polynomial given in (1.5) can lie outside the circle of radius $2 \max_{0 \leq j < n-1} |a_j|^{1/2}$ in the complex plane. Consider now the polynomial in (1.1) with $|b| < 1$, but $2|b| \geq 1$, and $(b + 1)/a > n - 1$. Then according to Case I.i.1 of Lemma 3.1, all the roots of $p_n(z)$ are in the interior of the unit circle. The result of Ostrowski in this case assures us only that there is a circle of radius $r \geq 1$ in which all the roots of (1.1) lie.

An example of the above is the recurrence relation which results from a repeated application of inside contractions steps in the Nelder–Mead algorithm when it is applied to the function $f(x_1, \ldots, x_n) = x_1^2 + \cdots + x_n^2$. In this case, according to (1.2), $b = -1/2$ and $a = 1/(2n)$, so that, by Lemma 3.1, all the roots of (1.1) are in the interior of the unit disk, while Ostrowski’s result only predicts them to be in the unit circle.

It is easily seen that the remarks which applied in the previous paragraph to justify that the roots of (1.1) for the case when $a$ and $b$ satisfy the requirements for the inside contraction operation can be used to deduce similar conclusions in the case that the coefficients of (1.1) satisfy the requirements for the outside contraction step given in (1.3).

In Lemma 3.1, we assumed that $(b + 1)/a \neq k$, $k = -1, 0, 1, 2, \ldots, n - 1$. We now ask: what happens in the limiting cases? We shall discuss the instances when
(b + 1)/a = −1 or n − 1 in the following section and the case when this ratio is 0 towards the end of this section. To analyze the remaining cases, namely when (b + 1)/a = k, k ∈ {1, . . . , n − 2}, let us first of all observe the following:

Lemma 3.4. The equation
\[ z^m - z^{m-1} - \ldots - z - 1 = 0 \]  

has no roots lying on the unit circle for \( m \geq 2 \).

Proof. We first note that for \( m \geq 2 \), \( z = 1 \) cannot be a solution of (3.4). Multiplying (3.4) by \( z - 1 \), we obtain the polynomial
\[ z^{m+1} - 2z^m + 1 = 0. \]  

Now if \( u \neq 1 \) is a root of (3.5) so that \( u^{m+1} + 1 = 2u^m \), we see that if, additionally, \( u \) is on the unit circle, then by the triangle inequality we must have that
\[ 2 = |u^{m+1}| + 1 \geq |u^{m+1} + 1| = 2|u^m| = 2. \]

This implies that \( u^{m+1} = 1 \). Hence we have that \( u^m = 1 \), which implies \( u = 1 \). \( \Box \)

Lemma 3.4 leads us to the following theorem:

Theorem 3.5. Suppose that \( a, b \in \mathbb{R}, a \neq 0, \) and \( (b + 1)/a = k \) for some \( 1 \leq k \leq n - 2 \).

When \( |b| < 1 \). The polynomial (1.1) has \( n - 1 \) roots in the interior of the unit disk and one root in its exterior.

When \( |b| > 1 \). The polynomial in (1.1) has one root in the interior of the unit disk and \( n - 1 \) roots in its exterior.

Proof. We consider the case when \( |b| < 1 \), the proof of case when \( |b| > 1 \) being similar.

Using Lemma 3.1, i.i.2 and a continuity argument, we need only show that \( p_n \) of (1.1) has no roots on the unit circle. Define
\[ q_n(z) = b z^n - az^{n-1} - \ldots - az + 1. \]

Then for \( |z| = 1, 1/z = \bar{z} \) so that
\[ |q_n(z)| = |z^n p_n(z^{-1})| = |p_n(\bar{z})| = |\bar{p}_n(z)| = |p_n(z)|. \]

Thus if \( z \) is a root of \( p_n \) with \( |z| = 1 \), then \( z \) is a root of \( q_n \) and therefore also a root of the polynomial
\[ p_n(z) - bq_n(z) = (1 - b^2)z \left( z^{n-1} - \frac{a}{b + 1} z^{n-2} - \ldots - \frac{a}{b + 1} z - \frac{a}{b + 1} \right). \]
Now \((b+1)/a = k\) and so
\[
p_n(z) - b q_n(z) = (1 - b^2) z \left( z^{n-1} - \frac{1}{k} z^{n-2} - \cdots - \frac{1}{k} z - \frac{1}{k} \right).
\]
Set
\[
\tilde{p}_{n-1}(z) := z^{n-1} - \frac{1}{k} z^{n-2} - \cdots - \frac{1}{k} z - \frac{1}{k}.
\]
We shall next show that \(\tilde{p}_{n-1}\) has no roots lying on the unit circle. To this end define
\[
\tilde{q}_{n-1}(z) := -\frac{1}{k} z^{n-1} - \frac{1}{k} z^{n-2} - \cdots - \frac{1}{k} z + 1
\]
and observe first that if \(z\) is a root of \(\tilde{p}_{n-1}\) with \(|z| = 1\), then it is a root of \(\tilde{q}_{n-1}\) and therefore it is also a root of \(\tilde{p}_{n-1} + \tilde{q}_{n-1}/k\). A straightforward calculation now gives that
\[
\tilde{p}_{n-1}(z) + \frac{1}{k} \tilde{q}_{n-1}(z)
\]
\[
= (1 - k^{-2}) z \left( z^{n-2} - \frac{1}{k-1} z^{n-3} - \cdots - \frac{1}{k-1} z - \frac{1}{k-1} \right).
\]
Continuing the process, we find that for \(p_n\) not to have a root on the unit circle is equivalent to the polynomial equation
\[
z^{n-k} - z^{n-k-1} - \cdots - z - 1 = 0
\]
also not to have roots on the unit circle. By Lemma 3.4, this last condition is true when \(k \leq n - 2\). Our proof is now complete. \(\square\)

In all previous results in this section we assumed that in (1.1), \(|b| \neq 1\). In our final result of this section we shall permit \(b = -1\), in which case \((b+1)/a = 0\), while the case \(b = 1\) will be considered in the following section.

**Theorem 3.6.** Consider the polynomial given in (1.1). Suppose that \(n \geq 2\) and that \(b = -1\).\(\quad\) (3.6)

(i) If \(a > 0\), then the polynomial in (1.1) has \(n - 1\) roots in the interior of the unit disk and one root in its exterior.

(ii) If \(a < 0\), then the polynomial in (1.1) has \(n - 1\) roots in the exterior of the unit disk and one in its interior.

**Proof.** We shall only prove here part (i) as the proof of part (ii) follows similarly.

Since \(b = -1\), the polynomial in (1.1) becomes
\[
p_n(z) = z^n - a z^{n-1} - \cdots - a z - 1.\] (3.7)

Using Lemma 3.1 I.i.2, I.ii.2, and continuity arguments, we only need to show that \(p_n\) has no roots lying on the unit circle. To this end, define
\[ q_n(z) = -z^n - az^{n-1} - \cdots - az + 1. \]

As in the proof of the previous theorem,
\[ |p_n(z)| = |q_n(z)| \]
for all \( z \) with \( |z| = 1 \). Now if \( z \) is a root of \( p_n \) with \( |z| = 1 \), then it is a root of \( q_n \) and therefore also a root of
\[ p_n(z) - q_n(z) = 2z^n - 2. \]
However, any root of \( 2z^n - 2 = 0 \) cannot be a root of the polynomial \( p_n(z) \) of (3.7) with \( n \geq 2 \). Hence \( p_n \) has no roots lying on the unit circle. \( \Box \)

4. The case of some zeros on the unit circle

In the previous section we were concerned with values of \( a \) and \( b \), satisfying the condition in (1.8), which ensure that the polynomial (1.1) has no roots on the unit circle. In this section we shall investigate real values of the parameters \( a \) and \( b \) which lead to roots of (1.1) on the unit circle. It will be shown that only one of the three following situations can occur: 1, or \( n - 1 \), or all of the roots of (1.1) can be on the unit circle.

We start with the case when \(|b| \neq 1\). We have the following theorem:

**Theorem 4.1.** Suppose that \( a, b \in \mathbb{R} \) and \( a \neq 0 \).

**Case I. Assuming that \(|b| < 1\):**

I(i) The polynomial in (1.1) has one root in the interior of the unit disk and the remaining roots on the unit circle if
\[ \frac{b + 1}{a} = -1. \]

I(ii) The polynomial in (1.1) has one root on the unit circle and the remaining roots in the interior of the unit disk if
\[ \frac{b + 1}{a} = n - 1. \]

**Case II. Assuming that \(|b| > 1\):**

II(i) The polynomial in (1.1) has one root in the exterior of the unit disk and the remaining roots on the unit circle if
\[ \frac{b + 1}{a} = -1. \]
The polynomial in (1.1) has one root on the unit circle and the remaining roots in the exterior the unit disk if

$$\frac{b + 1}{a} = n - 1.$$  

**Proof.** We prove Case I. The proof of Case II follows similarly.

**Case I(i).** Since $\left(\frac{b + 1}{a}\right) = -1$, the equation $b - az - \cdots - az^{n-1} + z^n = 0$ reduces to

$$z^n - 1 - a(z^{n-1} + \cdots + z + 1) = 0,$$

or

$$(z - a - 1)(z^{n-1} + \cdots + z + 1) = 0.$$  

This polynomial has a root $z = a + 1 = -b$ in the interior of the unit disk and $n - 1$ roots on the unit circle.

**Case I(ii).** Let $p_n(z)$ be as in (1.1). Using Lemma 3.1, Case I.i.1 and a continuity argument, we conclude that all the roots of $p_n$ lie in the interior of the unit disk. The condition that $(b + 1)/a = n - 1$ implies that $p_n$ has a root $z = 1$ on the unit circle. We shall show that the remaining $n - 1$ roots lie in the interior of the unit disk. Define

$$q_n(z) = 1 - az - \cdots - az^{n-1} + bz^n.$$  

Then if $|z| = 1$, we have that

$$1/z = \bar{z},$$  

and, moreover,

$$|q_n(z)| = |z^n p_n(z^{-1})| = |p_n(\bar{z})| = |p_n(z)| = |p_n(z)|.$$  

Thus, if $w$ is a root of $p_n$ with $|w| = 1$, then it is also a root of $q_n$ and therefore a root of $p_n - bq_n$. Consider the difference

$$p_n(w) - bq_n(w) = (1 - b^2)w \left( w^{n-1} - \frac{a}{b + 1}w^{n-2} - \cdots - \frac{a}{b + 1}w - \frac{a}{b + 1} \right).$$  

Substituting $(b + 1)/a = n - 1$ gives that

$$p_n(w) - bq_n(w) = (1 - b^2)w \left( w^{n-1} - \frac{1}{n - 1}w^{n-2} - \cdots - \frac{1}{n - 1}w - \frac{1}{n - 1} \right).$$  

This polynomial has a root $w = 0$ lying inside the unit disk. Its other $n - 1$ roots are the solutions of the equation

$$w^{n-1} - \frac{1}{n - 1}w^{n-2} - \cdots - \frac{1}{n - 1}w - \frac{1}{n - 1} = 0.$$  

(4.1)
The companion matrix of (4.1) is
\[
\begin{pmatrix}
\frac{1}{n-1} & \frac{1}{n-1} & \cdots & \frac{1}{n-1} & \frac{1}{n-1} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{pmatrix}_{(n-1) \times (n-1)}
\]

Note that this matrix is nonnegative and primitive (see, for example, Problem 5 [4, p. 522]). By the Perron–Frobenius theory for nonnegative matrices (see, for example, [4]), it has an eigenvalue $\lambda = 1$ and the remaining $n-2$ eigenvalues with modulus less than 1. Thus equation (4.1) has a root $w = 1$ on the unit circle and $n-2$ roots in the interior of the unit disk. Thus $p_n - bq_n$ has exactly one root lying on the unit circle. This implies that $p_n$ has exactly one root on the unit circle and $n-1$ roots in the interior the unit disk. \(\square\)

We comment that the above theorem can also be proved by checking that the conditions given in Theorem 44.1 of [8] for the polynomial (1.1) with two parameters hold.

Now we consider the case when $b = 1$. We have the following result:

**Theorem 4.2.** Consider the polynomial given in (1.1). If
\[
b = 1
\]
and
\[
0 \leq a \leq \frac{2}{n-1},
\]
then all roots of the polynomial (1.1) are on the unit circle.

**Proof.** Given $\epsilon > 0$ suppose that $0 \leq a < 2/(n-1) - \epsilon$. For such a fixed $a$, consider two sequences $\{b_1^{(j)}\}$ and $\{b_2^{(j)}\}$ of numbers satisfying that $b_1^{(j)} \uparrow 1$ and $b_2^{(j)} \downarrow 1$, respectively. These choices imply that
\[
0 \leq a < \frac{b_1^{(j)} + 1}{n-1}
\]
and
\[
0 \leq a < \frac{b_2^{(j)} + 1}{n-1}
\]
for all sufficiently large $j$.

Construct two sequences of polynomials:
\[
p_1^{(j)}(z) = z^n - a z^{n-1} - \cdots - a z + b_1^{(j)}, \quad j \geq 1,
\]

\[
p_2^{(j)}(z) = z^n - a z^{n-1} - \cdots - a z + b_2^{(j)}, \quad j \geq 1.
\]
and
\[ p_2^{(j)}(z) = z^n - az^{n-1} - \cdots - az + b^{(j)}, \quad j \geq 1. \] (4.5)

We know from Lemma 3.1 that for all sufficiently large \( j \), all roots of \( p_1^{(j)} \) are in the interior of the unit disk and all roots of \( p_2^{(j)} \) are in the exterior of the unit disk.

We note that
\[ b_1^{(j)} - b_2^{(j)} \to 0 \quad \text{as} \quad j \to \infty. \]

By using, for example, theorem [4, p. 539] on the “continuous dependence of the zeros of a polynomial on its coefficients”, we can conclude that all roots of the polynomial
\[ z^n - az^{n-1} - \cdots - az + 1 \]
for \( 0 \leq a < 2/(n - 1) - \epsilon \). The proof is completed by letting \( \epsilon \to 0 \). □

Remark 4.3. Consider the application of (1.6) to the polynomial in (1.1) when \( b = 1 \) and \( 0 \leq a < 2/(n - 1) - 0 \). By Theorem 4.2, all the roots of (1.1) are on the unit circle. However, on using Theorem 3.6(i) in combination with (1.6) we can only infer that the polynomial (1.1) has roots whose smallest modulus is not less than the smallest positive root of the polynomial
\[ -1 + az + \cdots + az^{n-1} + z^n \]
which is known to be (by Theorem 3.6) in the interior of the unit disk.

An example of the above is the recurrence relation which results from a repeated application of reflection steps in the Nelder–Mead algorithm when it is applied to the function
\[ f(x_1, \ldots, x_n) = x_1^2 + \cdots + x_n^2. \]
In this case, according to (1.4), \( b = 1 \) and \( a = 2/n \), so that Theorem 4.2 tells us that all roots of the polynomial in (1.1) are on the unit circle.

5. Some properties of the roots as \( n \) increases

In this section we consider how the roots of the characteristic polynomials for inside contraction and outside contraction behave as \( n \) increases. Let \( z_{OC}(n) \) or \( z_{IC}(n) \) be a root of the polynomial (1.1) with \( a \) and \( b \) satisfying (1.3) or (1.2) respectively. Our first result shows that \( z_{OC}(n) \) and \( z_{IC}(n) \) converge to the boundary of the unit circle as \( n \to \infty \).

Theorem 5.1. For the roots \( z_{OC}(n) \) and \( z_{IC}(n) \) as defined above:
\[ \lim_{n \to \infty} |z_{OC}(n)| = 1 \] (5.1)
and
\[ \lim_{n \to \infty} |z_{IC}(n)| = 1. \] (5.2)

Proof. Since \( z = 1 \) is not a root of the polynomial (1.1) with \( a \) and \( b \) satisfying (1.3), we can rewrite (1.1) and (1.3) as
\[ (2z^n + 1) = \frac{3}{n} \frac{z - z^n}{1 - z}. \] (5.3)
If (5.1) does not hold, then by Lemma 3.1, there exists a constant $\epsilon$ and a subsequence $\{n_k\}$ such that

$$|z_{OC}(n_k)| \leq 1 - \epsilon.$$ 

Therefore,

$$|1 - z_{OC}(n_k)| \geq \epsilon.$$ 

Substituting $z_{OC}(n_k)$ in (5.3) gives that

$$\left(2z_{OC}(n_k)^{n_k} + 1\right) = \frac{3}{n_k} \frac{z_{OC}(n_k) - z_{OC}(n_k)^{n_k}}{1 - z_{OC}(n_k)}.$$ 

As $n_k \to \infty$, the left-hand side of the above equation converges to 1. However, the right-hand side converges to 0. This is a contradiction. Thus (5.1) holds.

Similarly, we can prove (5.2). □

In some instances we can refine the results of the above theorem. Let $\rho_{IC}(n)$ denote the largest modulus of the roots of the characteristic polynomial for inside contraction ((1.1) plus (1.2)). Our next result shows $\rho_{IC}(n)$ is an increasing function of $n$ which tends monotonically to 1 as $n \to \infty$. To prove this fact, we need the following lemma which is adapted from Lemma 3 in [2].

**Lemma 5.2** (Elsner et al. [2]). Let $a_i, b_i, i = 1, 2, \ldots, n$, be nonnegative numbers such that

$$\sum_{i=1}^{j} a_i \leq \sum_{i=1}^{j} b_i, \quad j = 1, 2, \ldots, n,$$

and consider the matrices

$$A = \begin{bmatrix} a_n & a_{n-1} & \cdots & a_2 & a_1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}$$

and

$$B = \begin{bmatrix} b_n & b_{n-1} & \cdots & b_2 & b_1 \\ 1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 & 0 \end{bmatrix}.$$ 

If $\rho(B) < 1$ and $b_1 > a_1 > 0$ then $\rho(A) < \rho(B)$, where $\rho(\cdot)$ denotes the spectral radius of a matrix.
We can now prove:

**Theorem 5.3.** \( \rho_{IC}(n) \) is an increasing function of \( n \).

**Proof.** By definition, \( \rho_{IC}(n) \) and \( \rho_{IC}(n+1) \) are the spectral radii of the nonnegative matrices

\[
A = \begin{bmatrix}
\frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{bmatrix}
\]

and

\[
B = \begin{bmatrix}
\frac{1}{2(n+1)} & \frac{1}{2(n+1)} & \cdots & \frac{1}{2(n+1)} & \frac{1}{2} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0
\end{bmatrix},
\]

respectively, where \( A \) is an \( n \times n \) matrix and \( B \) is an \( (n+1) \times (n+1) \) matrix. Then by Lemma 3.1, \( \rho(A) < 1 \), \( \rho(B) < 1 \). Define

\[
A_{\epsilon} = \begin{bmatrix}
\frac{1}{2n} & \frac{1}{2n} & \cdots & \frac{1}{2n} & \frac{1}{2} \\
1 & 0 & \cdots & 0 & 0 \\
0 & 1 & \cdots & 0 & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \cdots & 1 & 0 \\
0 & 0 & \cdots & 0 & 1
\end{bmatrix}_{(n+1) \times (n+1)}
\]

Since \( A \) is a submatrix of \( A_{\epsilon} \), by the Perron–Frobenius theory we have that \( \rho(A_{\epsilon}) \geq \rho(A) \) for any \( \epsilon > 0 \). Let \( a_1 = \epsilon, a_2 = 1/2, a_3 = \cdots = a_{n+1} = 1/(2n), b_1 = 1/2, \) and \( b_2 = \cdots = b_{n+1} = 1/(2(n+1)) \). Then \( a_1 < b_1 \) and

\[
\sum_{i=1}^{j} a_i \leq \sum_{i=1}^{j} b_i, \quad j = 1, 2, \ldots, n+1,
\]

if \( \epsilon \) is sufficiently small, say \( \epsilon < 1/(2n(n+1)) \). By Lemma 5.2 we conclude that \( \rho(A_{\epsilon}) < \rho(B) \). Therefore,

\[
\rho_{IC}(n) \leq \rho_{IC}(n+1).
\]

We close the paper by raising the following conjecture. Let \( \rho_{OC}(n) \) and \( \omega_{OC}(n) \) denote the largest and smallest moduli of the roots of the characteristic polynomial
for outside contraction ((1.1) plus (1.3)) respectively. Let $\omega_{IC}(n)$ denote the smallest modulus of the roots of the characteristic polynomial for inside contraction ((1.1) plus (1.2)). Then we have:

**Conjecture 5.4.** $\rho_{OC}(n)$ and $\omega_{IC}(n)$ are increasing functions of $n$ for $n \geq 1$ and $\omega_{OC}(n)$ is an increasing function of $n$ for $n \geq 15$.

We comment that our numerical results for $1 \leq n \leq 200$ show that this conjecture is true.

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**References**


